Nuclear Structure Libraries for LAHET^{TM} and MCNPX^{TM}

R. E. Prael
Group X-CI
Los Alamos National Laboratory

W. B. Wilson
Group T-2
Los Alamos National Laboratory

Submitted to: *Proceedings of the 4th Workshop on Simulating Accelerator Radiation Environments, Sept. 13-16, 1998, Knoxville, TN* (1998).

Abstract

A new data library was created for use in the gamma emission module used in LAHET3 and MCNPX. Modifications to existing methods were made to improve the estimation of the population of metastable states. A preliminary comparison was made of the new data library to the contents of the CINDER'90 data library to assess the feasibility of using calculated metastable state populations as input in CINDER'90 calculations.

Introduction

In the original release of the LAHET Code System (LCS)[1], the PHT code is used to create a gamma source file from the output of a LAHET execution. It includes gamma production both from π^0decay and from nuclear deexcitation following particle emission. Such a gamma source file[2] may be input to MCNP[3] for transport. Recent development has included PHT as a code package within LAHET3 and MCNPX[4], with gamma production treated equivalently to other particle production.

The original nuclear data library (PHTLIB) used for gamma emission with PHT was created from the LLNL CDRL79 library[5]. For deexcitation of a nucleus after nucleon and ion emission is terminated, the emission process in PHT follows branching ratios from PHTLIB where known, including internal transitions, stopping at delayed particle emission (β, α, or nucleon) or electron capture. The PHT module uses spin and parity information in PHTLIB to calculate branching in the gamma cascade when branching ratios are not available.

In the original implementation, all gamma emission and internal transition was allowed, with the time variable for the emitted gamma sampled using the known $t_{1/2}$ when available. It was assumed that the time evolution of the gamma burst, including a delayed gamma component, would be followed with MCNP using time cutoff and binning. In addition, an interface was developed to pass final state information to the CINDER'90[6] and ORIHET codes to follow time-dependent decay.

Recent applications of LAHET have emphasized the calculation of the production of residual nuclei and the source for decay-chain calculations with CINDER'90. To improve these calculations, three efforts have been undertaken.

- Modify PHT to terminate the gamma emission process at nuclear levels with $t_{1/2}$ exceeding a cutoff value to provide a well-defined metastable state production rate for CINDER'90.
- Create a contemporary data library to replace the original PHT data library (PHTLIB/CDRL) which contains current nuclear level structure and decay properties.
- Provide a new scheme to define the correspondence between a residual excited state produced from the PHT module and a known level in the CINDER'90 data library.

Initial Steps

The original PHTLIB/CDRL was modified to block the emission process based on a $t_{1/2}$ cutoff of 1 ms to test the method of producing metastable state input to CINDER'90 and to provide a reference point for new library development. This was accomplished by the simple modification of decay channel identifiers to a form not recognized by PHT for all levels with $t_{1/2} > 1$ ms. Testing employed LAHET2.8 followed by an execution of PHT with the modified PHTLIB/CDRL to estimate the production rates for metastable states with $t_{1/2} > 1$ ms.

The BUDAPEST_LEVELS.DAT file, compiled by G. Molnar *et al.*, was obtained from the RIPL project library[7] to explore the feasibility of creating a new PHT data library. Considerable effort was expended in translating to a Fortran-readable form for processing into PHTLIB format. The procedure described above was again used to prevent decay from states with $t_{1/2} > 1$ ms. A preliminary comparison of the new library (PHTLIB/RIPL) with the contents of the CINDER'90 library indicated that data for many isotopes was completely absent in the BUDAPEST_LEVELS.DAT file. To improve the match with the CINDER'90 library, data for 45 isotopes was copied from PHTLIB/CDRL to PHTLIB/RIPL; the library so modified and discussed below is identified as PHTLIB/SPEC0.

Having constructed the preliminary PHTLIB/SPEC0 library, a comparison was made between the excited states in the new PHTLIB/SPEC0 and the CINDER'90 library to check for inconsistencies and test the feasibility of establishing a correspondence table. Since the CINDER library does not contain the level excitation energy, a match in levels was assumed to be determined by closeness of the half-life values.

Notes on Comparison

The initial comparison was made only for excited states with $t_{1/2} > 1$ ms. For a very large percentage of levels, a 1-to-1 correspondence between the PHTLIB/SPEC0 and CINDER'90 levels was shown, matching half-lives fairly closely. Missing levels in PHTLIB are not a functional problem, but some large ranges of are missing in the RIPL data, particularly near Z=55. A few well-documented levels are missing from the current CINDER'90 library; these should be supplied if a calculated final-state population is to be fully treated by CINDER. In addition, there are many multiple unresolved levels in the RIPL-based data that must map to a single level in the CINDER'90 library.

In the following annotated table, parts of this level-by-level comparison are shown to illustrate these conclusions.

```
------------------------------------------------------------------

   Metastables States SPEC0 Library   Metastable States CINDER Library
         (T-half >= 1.0E-04)                (T-half >= 1.0E-04)

------------------------------------------------------------------

   Z    A   I   E-lev     T-half            Z    A   I    T-half
   39   86  1  0.21830  2.8800E+03    |    39   86   1  2.8800E+03
   39   87  1  0.38079  4.8130E+04    |    39   87   1  4.6400E+04
   39   88  2  0.67455  1.3900E-02    |
   39   89  1  0.90896  1.6060E+01    |    39   89   1  1.6060E+01
   39   90  1  0.68203  1.1680E+04    |    39   90   1  1.1484E+04
   39   91  1  0.55558  2.9830E+03    |    39   91   1  2.9826E+03
   39   93  1  0.75872  8.2000E-01    |    39   93   1  8.2000E-01
   39   96  1  0.00100  6.0000E+00 a  |    39   96   1  9.6000E+00
                                      |    39   96   2  1.0000E-01
   39   97  1  0.66751  1.1700E+00    |    39   97   1  1.2300E+00
   39   97  2  3.52330  1.4200E-01    |
   39   98  1  0.00100  2.0000E+00 a  |    39   98   1  2.0000E+00
                                      |    39  100   1  9.4000E-01
                                      |    40   83   1  7.0000E+00
```

40	85	1	0.29220	1.0900E+01		|	40	85	1	1.0900E+01
40	87	1	0.33573	1.4000E+01		|	40	87	1	1.4000E+01
40	89	1	0.58784	2.5080E+02		|	40	89	1	2.5080E+02
40	90	1	2.31900	8.0920E-01		|	40	90	1	8.0920E-01
41	87	1	0.00100	1.5600E+02	a	|	41	87	1	2.2900E+02
41	88	1	0.00100	8.5800E+02	a	|	41	88	1	4.6800E+02
41	89	1	0.00100	7.2000E+03	a	|	41	89	1	3.9600E+03
41	90	1	0.12467	1.8810E+01		|	41	90	1	1.8820E+01
41	90	2	0.38201	6.1900E-03		|				
41	91	1	0.10449	1.2700E+06		|	41	91	1	5.3568E+06
41	92	1	0.13550	2.1180E+05		|	41	92	1	8.7696E+05

In the above examples, several levels from the CDRL data (indicated by the label *a*) have been included; the match in $t_{1/2} >$ is not generally good. Levels with fairly short half-lives are missing from both libraries.

49	123	1	0.32000	4.7800E+01	c	|	49	123	1	4.7800E+01
49	123	2	0.32700	4.7800E+01	c	|				
49	124	1	0.19000	3.4000E+00		|	49	124	1	2.4000E+00
49	125	1	0.18000	1.2200E+01	c	|	49	125	1	1.2200E+01
49	125	2	0.36000	1.2200E+01	c	|				
49	126	1	0.10200	1.6400E+00		|	49	126	1	1.5000E+00
49	127	1	0.46200	3.6700E+00		|	49	127	1	3.7600E+00
49	128	1	0.08000	7.0000E-01	c	|	49	128	1	9.0000E-01
49	128	2	0.32000	7.2000E-01	c	|				
49	129	1	0.20000	1.2300E+00	c	|	49	129	1	1.2600E+00
49	129	2	0.38000	1.2300E+00	c	|				
49	130	1	0.05000	5.5000E-01		|	49	130	1	5.5000E-01
49	130	2	0.40000	5.4200E-01		|	49	130	2	5.5000E-01

Above are four pairs of levels in the PHTLIB/SPEC0, labeled *c*, which apparently map into single levels in the CINDER library.

53	134	1	0.31649	2.1600E+02		|	53	134	1	2.2140E+02
53	136	1	0.64000	4.6900E+01		|	53	136	1	4.6900E+01
						|	54	111	1	9.0000E-01
54	125	1	0.25280	5.7000E+01		|	54	125	1	5.7000E+01
54	127	1	0.29720	6.9000E+01	a	|	54	127	1	6.9200E+01
54	129	1	0.23614	1.8530E+05		|	54	129	1	7.6810E+05
54	131	1	0.16393	2.4900E+05		|	54	131	1	1.0282E+06
54	132	1	2.75227	8.3900E-03		|				

54	133	1	0.23322	4.5690E+04	54	133	1	1.8922E+05
54	134	1	1.96550	2.9000E-01	54	134	1	2.9000E-01
54	135	1	0.52655	9.1740E+02	54	135	1	9.1740E+02
					54	143	1	3.0000E-01
					55	116	1	6.9000E-01
					55	117	1	8.5000E+00
					55	118	1	1.7000E+01
					55	119	1	2.8000E+01
					55	120	1	6.0000E+01
					55	121	1	1.2000E+02
					55	122	1	2.7000E+02
					55	122	2	3.6000E-01
55	123	1	0.15674	1.6400E+00	55	123	1	1.6000E+00
55	124	1	0.46254	6.3000E+00	55	124	1	6.3000E+00
55	130	1	0.16325	2.0760E+02	55	130	1	2.0800E+02
55	134	1	0.13874	1.0450E+04	55	134	1	1.0476E+04
55	135	1	1.63290	3.1800E+03	55	135	1	3.1800E+03
					55	136	1	1.9000E+01
55	138	1	0.07990	1.7460E+02	55	138	1	1.7460E+02
					56	125	1	7.8120E+03
56	127	1	0.08033	1.9000E+00				
56	129	1	0.00842	7.8120E+03	56	129	1	7.8120E+03
56	130	1	2.47512	1.1000E-02	56	130	1	1.1000E-02

In the above passage, a large range of missing data occurs in the RIPL-based data. In addition, note the few cases with very large discrepancies in $t_{1/2}$ that must be resolved.

Conclusions

Overall, it appears feasible to create a mapping of level data in the RIPL-based PHTLIB to levels in the CINDER library specifying calculated metastable state populations as input to CINDER. However, it is also apparent that considerable effort must be expended, in adding and modifying data in both libraries, to achieve that result. Adding data from the CDRL79 library is not always successful since there is frequently too large a discrepancy with current data.

Similar effort must be directed toward the states with $t_{1/2} < 1$ ms. However, since the gamma-emitting states will *not* appear as final states in the present computational scheme, the number of levels that must be matched is considerably smaller.

References

[1] Richard E. Prael and Henry Lichtenstein, "User Guide to LCS: The LAHET Code System", LA-UR-89-3014, Los Alamos National Laboratory (September 1989).
http://www-xdiv.lanl.gov/XCI/PROJECTS/LCS/lahet-doc.html

[2] Richard E. Prael, "Upgrade Package for LCS with LAHET2.7", LA-UR-97-4981 (December 1997)
http://www-xdiv.lanl.gov/XCI/PROJECTS/LCS/upgrade-doc.html

[3] Judith F. Briesmeister, editor, "MCNP^{TM} - A General Monte Carlo N-Particle Transport Code", Los Alamos National Laboratory report LA-12625-M (March 1997).
http://www-xdiv.lanl.gov/XCI/PROJECTS/MCNP/manual.html

[4] H. G. Hughes, et al., "The MCNP/LCS Merger Project", *Topical Meeting on Nuclear Applications of Accelerator Technology*, Albuquerque, NM, November 1997, p. 213, American Nuclear Society, La Grange Park, Illinois (1997).

[5] R. J. Howerton, "ENSL and CDRL: Evaluated Nuclear Structure Libraries", UCRL-50400, Vol. 23, Lawrence Livermore National Laboratory (February 1981).

[6] W. B. Wilson *et al.*, "Cinder'90 Code for Transmutation Calculations", *Proceedings of the International Conference on Nuclear Data for Science and Technology, Trieste, 19-24 May 1997*, Italian Physical Society, Bologna (1997).
http://t2.lanl.gov/publications/trieste97.html

[7] M. B. Chadwick *et al.*, "Reference Input Parameter Library: Handbook for Calculations of Nuclear Reaction Data", IAEA-TECDOC-Draft, IAEA, Vienna (March 1998).
http://iaeand.iaea.or.at/ripl/